CHEMICALS

Project Fact Sheet

Solution Crystallization Modeling Tools

Benefits

- Improved product quality in terms of crystal size purity
- Reduced losses, rework and downtime
- Shortened new product development time
- Improved filterability and mixing efficiency
- Energy savings of 12 trillion BTU per year

Applications

The new software tools to predict and optimize crystallization processes can be applied throughout the chemical and pharmaceutical industry. Some examples include bulk chemicals and salts, catalyst materials, ceramic powders, magnetic media, environmental wastewater cleanup, fertilizers, building materials, and drugs.

Software Tools Will Optimize Crystallization Processes

Crystallization processes could be more effective, economical, and energy efficient if accurate software design and process modeling tools were available. Crystallization is the most widely used separation and purification process employed throughout the chemical and pharmaceutical industry for chemical products that are solids at room temperature and pressure. Today, crystallization modeling tools are limited by the availability of methods to reliably predict solubility and supersaturation for chemical systems of industrial importance. There is also limited capability for describing nucleation, growth, particle agglomeration and attrition, and mixing and design scale-up for industrial crystallizers. Tools are needed to model and optimize crystallizer process performance with respect to product quality, throughput, and efficiency.

Project partners will directly address these limitations by developing software tools to predict supersaturation and simulate commercial crystallization unit operations. Computational fluid dynamics will be used to analyze and design crystallizer vessels based on phenomenological models for nucleation, growth, and particle agglomeration and attrition. These new software tools will help design crystallizers with improved product quality, minimum product loss, maximum energy efficiency and reduced product manufacturing time. By 2020, adoption of improved crystallizers could yield energy savings of 12 trillion BTU per year.

Crystal Formation

New models will simulate crystal nucleation, growth, agglomeration and attrition in commercial-scale crystallizers.

Project Description

Goal: To develop software tools for analyzing and optimizing crystallizer separation hardware and processes.

OLI Systems is a world leader in supplying process chemistry and thermodynamics software products to the chemical process industry. Fluent Inc. is a leading supplier of computational fluid dynamics (CFD) software to the chemical process and other industries. The OLI thermodynamic model is currently in use by over 75 companies around the world. As a basis for this thermodynamic framework, over a thousand potential solids, as well as their solution species, are currently contained in the OLI Databank. Expansion of the Databank to include more ionic and non-ionic solids for aqueous and mixed solvent systems is necessary to provide a comprehensive Databank for industrial use.

Once the basic level of physical properties and thermodynamics is established, the next level of crystallization phenomenology becomes practical. Supersaturation is the primary driving force in crystallization and its prediction is crucial to further development of crystallization kinetics models. Further development of crystallization phenomena modeling is necessary in the areas of nucleation and growth, aggregation and agglomeration, breakage, and fines destruction. The addition of these kinetics phenomena, linked with the rigorous thermodynamics model, will provide improved accuracy in predicting the crystal mass and area which is necessary to perform engineering analysis at the process level, and, coupled to Fluent's CFD models, at the crystallizer level.

Progress & Milestones

Work is now progressing on the development and refinement of a solubility database and thermodynamic model, the particle kinetics models, and the micro-mixing (CFD) models. Future research will focus on achieving the following milestones:

- Develop a comprehensive solubility data base, mixed solvent thermodynamic framework, and supersaturation prediction capability in software tools for crystallization systems of priority interest to the U.S. chemical process industry
- Design software for commercial crystallization unit operations and process simulation
- Create detailed computational fluid dynamics crystallizer hardware design and optimization software
- Test and validate the models using real crystallization plant systems data
- Produce easy-to use software tools that allow the engineer or scientist to access the above capabilities without a major investment of time in learning to use the software.

Commercialization

Two commercial software products that will allow industry to predict and optimize the performance of real industrial crystallization processes, CrystalAnalyzer™ for crystallization chemistry and process analysis, and CrystalSimulator for CFD crystallizer design analysis, will be marketed.

Project Partners

OLI Systems
Morris Plains, NJ

Fluent
Lebanon, NH

For additional information, please contact:

Charles Russomanno
Office of Industrial Technologies
Phone: (202) 586-7543
Fax: (202) 586-1658
charles.russomanno@ee.doe.gov

Please send any comments, questions, or suggestions to
webmaster.oit@ee.doe.gov

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Office of Industrial Technologies
Energy Efficiency
and Renewable Energy
U.S. Department of Energy
Washington, D.C. 20585

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